Molecular Ro-vibrational Collision Rates for Infrared Modeling of Warm Interstellar Gas from Full-dimensional Quantum Calculations

Completed Technology Project (2016 - 2020)

Project Introduction

We propose to compute accurate collisional excitation rate coefficients for rovibrational transitions of CS, SiO, SO, NO, H_2O, and HCN due to H_2, He, or H impact. This extends our previous grant which focused on 3- and 4-atom systems to 4- and 5-atom collision complexes, with dynamics to be performed on 6-9 dimensional potential energy surfaces (PESs). This work, which uses fully quantum mechanical methods for inelastic scattering and incorporates full-dimensional PESs, pushes beyond the state-of-the-art for such calculations, as recently established by our group for rovibrational transitions in CO-H_2 in 6D. Many of the required PESs will be computed as part of this project using ab initio theory and basis sets of the highest level feasible and particular attention will be given to the long range form of the PESs. The completion of the project will result in 6 new global PESs and state-to-state rate coefficients for a large range of initial rovibrational levels for temperatures between 1 and 3000 K. The chosen collision systems correspond to cases where data are limited or lacking, are important coolants or diagnostics, and result in observable emission features in the infrared (IR). The final project results will be important for the analysis of a variety of interstellar and extragalactic environments in which the local conditions of gas density, radiation field, and/or shocks drive the level populations out of equilibrium. In such cases, collisional excitation data are critical to the accurate prediction and interpretation of observed molecular IR emission lines in protoplanetary disks, star-forming regions, planetary nebulae, embedded protostars, photodissociation regions, etc. The use of the proposed collisional excitation data will lead to deeper examination and understanding of the properties of many astrophysical environments, hence elevating the scientific return from the upcoming JWST, as well as from current (SOFIA, Herschel, HST) and past IR missions (Spitzer, ISO), and from ground-based telescopes.

Molecular Ro-vibrational Collision Rates for Infrared Modeling of Warm Interstellar Gas from Full-dimensional Quantum Calculations

Table of Contents

Organizational Responsibility

Responsible Mission Directorate:

Science Mission Directorate (SMD)

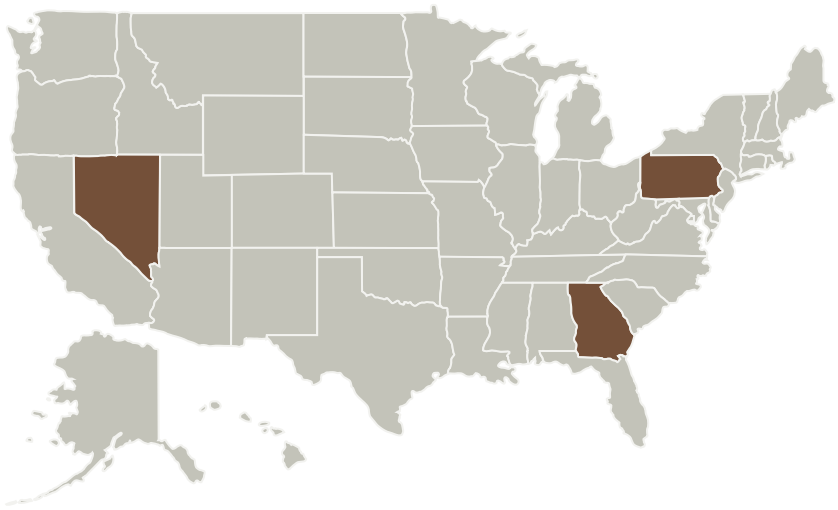
Responsible Program:

Astrophysics Research and Analysis

Molecular Ro-vibrational Collision Rates for Infrared Modeling of Warm Interstellar Gas from Full-dimensional Quantum Calculations

Completed Technology Project (2016 - 2020)

Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
University of Georgia Research Foundation, Inc.	Supporting Organization	Academia	Athens, Georgia

Primary U.S. Work Locations	
Georgia	Nevada
Pennsylvania	

Project Management

Program Director:

Michael A Garcia

Program Manager:

Dominic J Benford

Principal Investigator:

Phillip C Stancil

Co-Investigators:

Benhui Yang
Robert C Forrey
Balakrishnan Naduvalath
Joel M Bowman
Cynthia Baker

Technology Areas

Primary:

- TX17 Guidance, Navigation, and Control (GN&C)
  - TX17.5 GN&C Systems Engineering Technologies
    - TX17.5.9 Onboard and Ground-BasedTerrain and Object Simulation, Mapping, and Modeling Software

Target Destination

Outside the Solar System